Hindawi Publishing Corporation
Advances in High Energy Physics
Volume 2014, Article ID 952597, 7 pages
http://dx.doi.org/10.1155/2014/952597

Hindawi

Research Article

Analytical Solution of the Schrödinger Equation with Spatially Varying Effective Mass for Generalised Hylleraas Potential

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Received 30 May 2014; Revised 19 July 2014; Accepted 21 July 2014; Published 11 August 2014

Academic Editor: Shi-Hai Dong

We have obtained exact solution of the effective mass Schrödinger equation for the generalised Hylleraas potential. The exact bound state energy eigenvalues and corresponding eigenfunctions are presented. The bound state eigenfunctions are obtained in terms of the hypergeometric functions. Results are also given for the special case of potential parameter.

1. Introduction

The study of quantum mechanical systems within the framework of effective position dependent mass has been the subject of much activity in recent years. The Schrödinger equation with position-dependent (nonconstant) mass provides an interesting and useful model for the description of many physical problems. The most extensive use of such an equation is in the physics of semiconductor nanostructures [1, 2], quantum dots [3], ^{3}He clusters [4], quantum liquids [5], semiconductor heterostructures [6, 7], and so forth.

The solutions of nonrelativistic wave equations with constant mass have been extended to the position dependent mass in recent studies [8–11]. A general formalism for energy spectra and wave functions was found in nonrelativistic problems by using point canonical transformation [8]. Compared to the constant mass wave equation, the position-dependent mass Schrödinger equation is more complex. It is difficult to obtain its analytical solution as usual. Several authors have studied the effects of the position-dependent mass on the solutions of the Schrödinger equation. A position-dependent effective mass, $m(x) = m_1 \cdot m(x)$, associated with a quantum mechanical particle constitutes a useful model for the study of various potentials such as Morse potential [12–18], hard-core potential [18], Scarf potential [19–21], Pöschl-Teller potential [22, 23], spherically ring-shaped potential [24], Hulthén potential [25], Kratzer potential [26], and Coulomb-like potential [27, 28]. Different techniques have been developed to obtain its exact solutions, such as factorization methods [29], Nikiforov-Uvarov (NU) methods [30], and supersymmetric quantum mechanics [31]. The position-dependent effective mass might have impact on high-energy physics [31].

The objective of this paper is to investigate the position-dependent effective mass Schrödinger equation for the generalised Hylleraas potential [32, 33] by using the Nikiforov-Uvarov (NU) method (Figure 1) [30]. Hylleraas potential is used to describe the interaction between two atoms in a diatomic molecule. We have also investigated the solutions of Hulthén potential and Woods-Saxon potential.

The plan of the present paper is as follows. In Section 2, the Nikiforov-Uvarov method is summarized. Section 3 is devoted to the solution of the position-dependent effective mass Schrödinger equation. In Sections 4 and 5, the Hulthén potential and Woods-Saxon potential are discussed, respectively. The paper is ended with a summary.

2. Nikiforov-Uvarov Method

The NU method is a useful technique to solve the second-order linear differential equations with special orthogonal functions [34]. In this method, after employing an appropriate coordinate transformation $s = s(x)$, the nonrelativistic

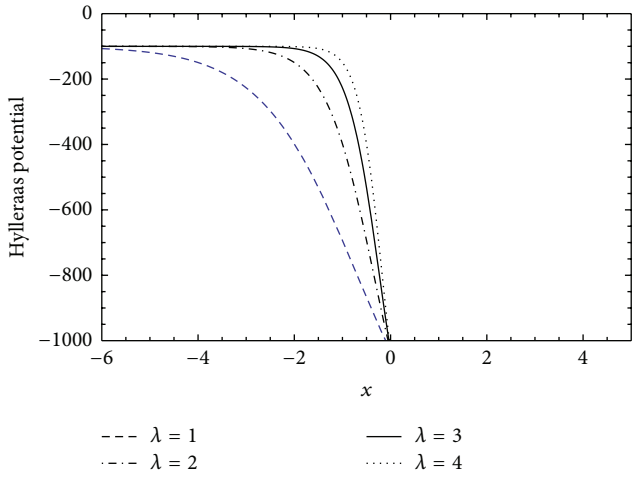

FIGURE 1: Hylleraas potential for $V_1 = 50$, $V_2 = 100$, $a = 10$, $b = 0.5$, and $d = 20$.

Schrödinger equation $d^2\psi/dx^2 + (E - V(x))\psi = 0$, ($\hbar = 2m = 1$) can be written in the following form:

$$\psi''(s) + \frac{\widetilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \tag{1}$$

where the prime denotes the differentiation with respect to s, $\sigma(s)$ and $\widetilde{\sigma}(s)$ are polynomials, at most of second degree, and $\widetilde{\tau}(s)$ is a polynomial, at most of first degree. In order to obtain a particular solution to (1), we set the following wave function as a multiple of two independent parts:

$$\psi(s) = \phi(s)\, y_n(s). \tag{2}$$

Equation (2) transformed (1) to a hypergeometric-type equation:

$$\sigma(s)\, y_n''(s) + \tau(s)\, y_n'(s) + \lambda y_n(s) = 0, \tag{3}$$

where first part of (2), $\phi(s)$, has a logarithmic derivative:

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \tag{4}$$

and second part of (2), $y_n(s)$, is the hypergeometric-type function whose polynomial solution satisfies the Rodrigues relation:

$$y_n(s) = \frac{C_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\,\rho(s)\right], \tag{5}$$

where C_n is normalization constant and the weight function $\rho(s)$ satisfies the relation as

$$\frac{d}{ds}\left[\sigma(s)\,\rho(s)\right] = \tau(s)\,\rho(s). \tag{6}$$

The function $\pi(s)$ and the eigenvalue λ required in this method are defined as

$$\pi(s) = \left(\frac{\sigma' - \widetilde{\tau}}{2}\right) \pm \sqrt{\left(\frac{\sigma' - \widetilde{\tau}}{2}\right)^2 - \widetilde{\sigma} + k\sigma}, \tag{7}$$

$$k = \lambda - \pi'(s). \tag{8}$$

Hence, the determination of k is the essential point in the calculation of $\pi(s)$, for which the discriminant of the square root in (7) is set to zero. Also, the eigenvalue equation defined in (8) takes the following new form:

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), \quad n = 0, 1, 2, \ldots, \tag{9}$$

$$\tau(s) = \widetilde{\tau}(s) + 2\pi(s), \quad \tau'(s) < 0. \tag{10}$$

Since $\rho(s) > 0$ and $\sigma(s) > 0$, the derivative of $\tau(s)$ should be negative [30], which helps to generate the essential condition for any choice of proper bound state solutions. In addition, the energy eigenvalues are obtained from (8) and (9).

3. Position-Dependent Effective Mass Schrödinger Equation

In general, working on position-dependent effective mass Hamiltonians is inspired by the von Roos Hamiltonian [35] proposal with $\hbar = 2m_0 = 1$:

$$\begin{aligned}\Big[-\frac{1}{2}\Big(&m^{\alpha}(x)\,\partial_x m^{\beta}(x)\,\partial_x m^{\gamma}(x) \\ &+ m^{\gamma}(x)\,\partial_x m^{\beta}(x)\,\partial_x m^{\alpha}(x)\Big) + V(x)\Big]\varphi(x) \\ &= E\varphi(x),\end{aligned} \tag{11}$$

where $\hbar = 2m_0 = 1$ and $m(x)$ is the dimensionless form of the function $m(x) = m_1 \cdot m(x)$. The ambiguity parameters are constrained by the relation $\alpha + \beta + \gamma = -1$ and we have the following time-independent Schrödinger equation from (11):

$$H\varphi(x) \equiv \left[-\partial_x\left(\frac{1}{m(x)}\right)\partial_x + V_{\text{eff}}(x) - E\right]\varphi(x) = 0, \tag{12}$$

where the effective potential is

$$\begin{aligned}V_{\text{eff}}(x) = V(x) &+ \frac{1}{2}(\beta+1)\frac{m''(x)}{m^2(x)} \\ &- \left[\alpha(\alpha+\beta+1) + (\beta+1)\right]\frac{m'^2(x)}{m^3(x)},\end{aligned} \tag{13}$$

where primes denote derivatives. Thus Schrödinger equation takes the form

$$\left(-\frac{1}{m(x)}\frac{d^2}{dx^2} + \frac{m'(x)}{m^2(x)}\frac{d}{dx} + V_{\text{eff}}(x) - E\right)\varphi(x) = 0. \tag{14}$$

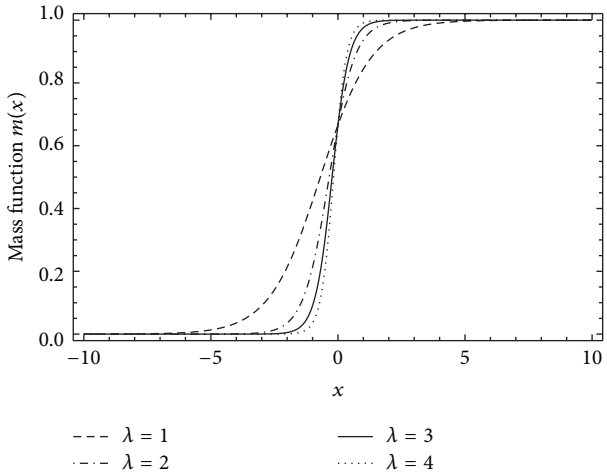

FIGURE 2: Plot for mass function $m(x)$ for $b = 0.5$ and $m_1 = 1$.

Using the transformation [36], $\varphi(x) = m^{\nu}(x)\psi(x)$ in (14), we have

$$\left\{-\frac{d^2}{dx^2} - (2\nu - 1)\frac{m'(x)}{m(x)}\frac{d}{dx} - \left(\nu(\nu-2) + \alpha(\alpha+\beta+1) + \beta + 1\right)\frac{m'^2}{m^2} + \left(\frac{1}{2}(\beta+1) - \nu\right)\frac{m''(x)}{m(x)} + m(x)(V(x) - E)\right\}\psi(x) = 0, \tag{15}$$

where $V(x)$ is the Hylleraas potential [29, 30] given by

$$V(x) = V_1\frac{a + e^{\lambda x}}{b + e^{\lambda x}} - V_2\frac{d + e^{\lambda x}}{b + e^{\lambda x}}, \tag{16}$$

where $a(\neq b)$, b, and $d(\neq b)$ are the Hylleraas parameters, V_1, V_2 are the potential depths, and $-\infty < x < \infty$.

Here, we consider the following mass distribution:

$$m(x) = \frac{m_1}{1 + be^{-\lambda x}}. \tag{17}$$

The most extensive use of such kind of mass is in the physics of semiconductor quantum well structures [11]. The motion of electrons in them can often be described by the envelope function effective-mass Schrödinger equation, where m_1 is a constant mass (Figure 2).

Obviously it has the exponential form. The above mass function is convergent $m(x) \to m_1$ (finite), when $x \to \infty$.

In order to reduce the above equation (15) into Nikiforov-Uvarov equation, we make the transformation $s = 1/(1 + be^{-\lambda x})$, $(0 \le s \le 1)$:

$$\begin{aligned} A &= \nu(\nu-2) + \alpha(\alpha+\beta+1) + \beta + 1,\\ B &= \left(\frac{1}{2}(\beta+1) - \nu\right),\\ \zeta &= \frac{1}{2} - \nu,\\ P - \zeta^2 &= -A + 2B - \frac{m_1(a-b)V_1}{b\lambda^2} + \frac{m_1(d-b)V_2}{b\lambda^2},\\ Q - 2\zeta^2 &= -2A + 3B - \frac{m_1(aV_1 - dV_2 - bE)}{b\lambda^2},\\ R - \zeta^2 &= -A + B,\\ P - Q + R &= \frac{m_1(V_1 - V_2 - E)}{\lambda^2} = \varepsilon^2; \end{aligned} \tag{18}$$

also

$$\begin{aligned} \frac{m'(x)}{m(x)} &= \lambda(1-s),\\ \frac{m''(x)}{m(x)} &= \lambda^2(1-s)(1-2s). \end{aligned} \tag{19}$$

Using (15)–(19), we have

$$\frac{d^2\psi}{ds^2} + \frac{2\nu - (2\nu+1)s}{s(1-s)}\frac{d\psi}{ds} + \frac{1}{s^2(1-s)^2}\left[\left(\zeta^2 - P\right)s^2 + \left(Q - 2\zeta^2\right)s + \left(\zeta^2 - R\right)\right]\psi = 0. \tag{20}$$

Comparing (20) with (1), we have

$$\begin{aligned} \sigma(s) &= s(1-s),\\ \widetilde{\sigma}(s) &= \left(\zeta^2 - P\right)s^2 + \left(Q - 2\zeta^2\right)s + \left(\zeta^2 - R\right),\\ \widetilde{\tau}(s) &= 2\nu - (2\nu+1)s. \end{aligned} \tag{21}$$

Substituting these polynomials into (7), we have

$$\pi(s) = \left(\frac{1}{2} - \nu\right)(1-s) \pm \begin{cases} \left(\sqrt{R} - \varepsilon\right)s - \sqrt{R}; & k = Q - 2R + 2\varepsilon\sqrt{R} \\ \left(\sqrt{R} + \varepsilon\right)s - \sqrt{R}; & k = Q - 2R - 2\varepsilon\sqrt{R}. \end{cases} \tag{22}$$

For physical solutions, it is necessary to choose

$$\pi(s) = \zeta(1-s) - \left(\sqrt{R} + \varepsilon\right)s + \sqrt{R} \quad \text{if } k = Q - 2R - 2\varepsilon\sqrt{R}. \tag{23}$$

The origin of the Nikiforov-Uvarov method is negative sign of derivative of $\tau'(s)$ because the condition $\tau'(s) < 0$ helps to generate energy eigenvalues and corresponding eigenfunctions. Therefore $\tau(s)$ becomes

$$\tau(s) = 1 + 2\sqrt{R} - 2\left(2 + 2\sqrt{R} + 2\varepsilon\right)s. \tag{24}$$

Therefore, from (8) and (9), we have

$$\begin{aligned} \lambda &= Q - 2R - 2\varepsilon\sqrt{R} - \zeta - \left(\sqrt{R} + \varepsilon\right), \\ \lambda &= \lambda_n = 2n\left(\sqrt{R} + \varepsilon\right) + n(n+1). \end{aligned} \tag{25}$$

Comparing (25), we have

$$\begin{aligned} \sqrt{R} + \varepsilon &= -\left(n + \frac{1}{2}\right) + \sqrt{P - \nu + \frac{1}{4}}, \\ \sqrt{R} - \varepsilon &= \frac{Q - P}{-(n + 1/2) + \sqrt{P - \nu + 1/4}}. \end{aligned} \tag{26}$$

Using (26) and (18), we have

$$\varepsilon^2 = \frac{1}{4}\left[2n + 1 + 2\sqrt{R} - \sqrt{P - \nu + \frac{1}{4}}\right]^2. \tag{27}$$

Hence the energy becomes

$$\begin{aligned} E_n &= -\frac{\lambda^2}{4m_1} \\ &\times \left[2n + 1 \right. \\ &\quad - 2\sqrt{\frac{m_1(V_1 - V_2)}{\lambda^2} - \frac{m_1(V_1 a - V_2 d)}{b\lambda^2} - \alpha(\alpha + \beta + 1)} \\ &\quad \left. + 2\sqrt{-\nu(\nu - 1) - \alpha(\alpha + \beta + 1) - \frac{(\beta + 1)}{2} + \left(\frac{1}{2} - \nu\right)^2}\right]^2 \\ &+ (V_1 - V_2), \quad 0 \le n < \infty. \end{aligned} \tag{28}$$

The last term of the square bracket must be positive for Ben-Daniel and Duke's model [37] ($\alpha = \nu = 0$, $\beta = -1$) (Figure 3).

From (6), (21), and (24) we obtain the weight function

$$\rho(s) = s^{2\sqrt{R}}(1 - s)^{2\varepsilon}, \tag{29}$$

and from (4), (21), and (23) we have

$$\phi(s) = s^{\sqrt{R} + \zeta}(1 - s)^{\varepsilon}. \tag{30}$$

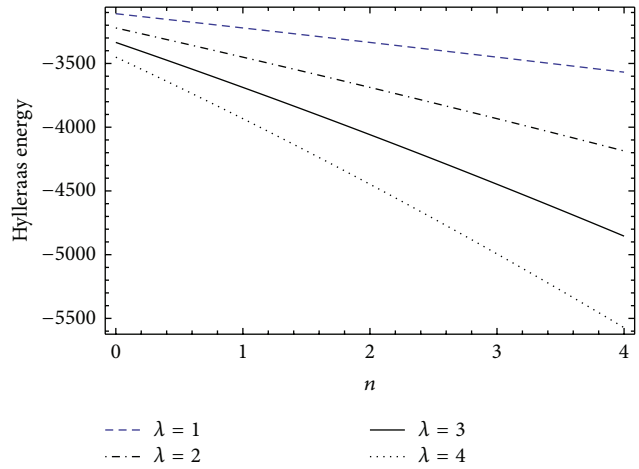

Figure 3: Hylleraas energy E_n for $\alpha = 0$, $\beta = -1$, $a = 10$, $b = 0.5$, $d = 20$, $m_1 = 1$, $V_1 = 50$, and $V_2 = 100$.

Now we use the properties of Jacobi polynomial [35]:

$$\begin{aligned} P_n^{(\zeta,\xi)}(x) &= \frac{(-1)^n(1 - x)^{-\zeta}(1 + x)^{-\xi}}{2^n n!} \\ &\times \frac{d^n}{dx^n}\left[(1 - x)^{n+\zeta}(1 + x)^{n+\xi}\right], \\ P_n^{(2\zeta,2\xi)}(1 - 2s) &= \frac{(-2)^n(s)^{-2\zeta}(1 - s)^{-2\xi}}{2^n n!} \\ &\times \frac{d^n}{dx^n}\left[s^{n+2\zeta}(1 - s)^{n+2\xi}\right], \end{aligned} \tag{31}$$

where $P_n^{(a,b)}(x)$ ($a > -1$, $b > -1$) is the Jacobi polynomial. The wave functions (Figure 4) are obtained from (2), (5), and ((29)–(31)):

$$\psi_n(s) = N_n s^{\sqrt{R}+\zeta}(1 - s)^{\varepsilon} P_n^{(2\sqrt{R},2\varepsilon)}(1 - 2s), \tag{32}$$

where N_n is normalization constant to be determined from the normalization condition:

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1 = \int_0^1 |\psi_n(s)|^2 ds. \tag{33}$$

For acceptable solution it is required that $|\sqrt{R} + \zeta| \ge \varepsilon$ when $\sqrt{R} + \zeta < 0$, $\varepsilon > 0$ and $\sqrt{R} + \zeta \le |\varepsilon|$ when $\sqrt{R} + \zeta > 0$, $\varepsilon < 0$.

4. Hulthén Potential

We set the conditions $V_2 = V_1$, $a = 1 + d$, and $b = -q$; the potential in (16) reduces to Hulthén potential (Figure 5) [38–41]:

$$V(x) = -V_1 \frac{e^{-\lambda x}}{1 - qe^{-\lambda x}}. \tag{34}$$

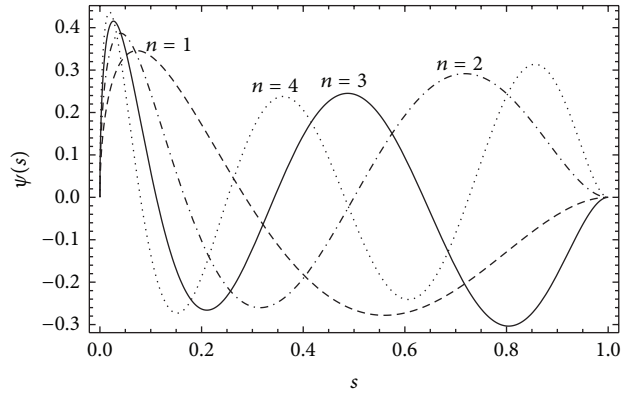

FIGURE 4: Wave functions $\psi_n(s)$ for $\alpha = 0$, $\beta = -1$, $\nu = 1/2$, and $\varepsilon = 2$.

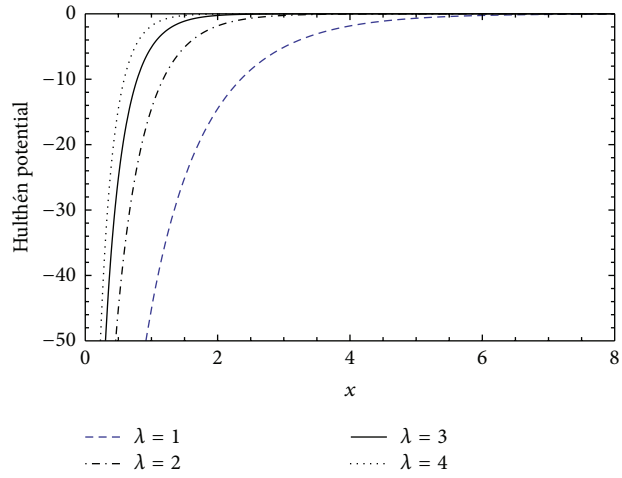

FIGURE 5: Hulthén potential for $V_1 = 100.0$ and $q = 0.5$.

Then the energy becomes

$$E_n = -\frac{\lambda^2}{4m_1} \times \left[2n + 1 - 2\sqrt{\frac{m_1 V_1}{q\lambda^2} - \alpha(\alpha+\beta+1)} + 2\sqrt{-\nu(\nu-1) - \alpha(\alpha+\beta+1) - \frac{(\beta+1)}{2} + \left(\frac{1}{2}-\nu\right)^2}\right]^2 \quad (35)$$

with $0 \le n < \infty$. It is exactly the same result in the literature [38] for $m_1 = 1$.

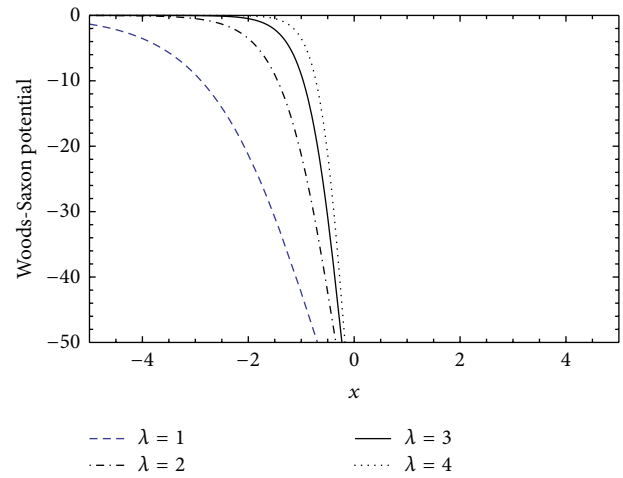

FIGURE 6: Woods-Saxon potential for $V_0 = 100.0$ and $b = 0.5$.

5. Woods-Saxon Potential

For the conditions $V_1 = -V_0$, $a = 0$, and $V_2 = 0$, the potential given in (16) becomes Woods-Saxon potential (Figure 6) [40–45],

$$V(x) = -V_0 \frac{1}{1 + be^{-\lambda x}}. \quad (36)$$

Then the energy becomes

$$E_n = -\frac{\lambda^2}{4m_1} \times \left[2n + 1 - 2\sqrt{\frac{m_1(1-b)V_0}{b\lambda^2} - \alpha(\alpha+\beta+1)} + 2\sqrt{-\nu(\nu-1) - \alpha(\alpha+\beta+1) - \frac{(\beta+1)}{2} + \left(\frac{1}{2}-\nu\right)^2}\right]^2 - V_0, \quad (37)$$

where $0 \le n < \infty$.

6. Conclusion

We have applied the NU method derived for the exponential-type potentials to obtain the bound state solutions of the effective Schrödinger equation with position-dependent mass for the Hylleraas potential. Furthermore, a suitable choice of a position mass function of the exponential-like form has also been devised. Also we have shown that our results are consistent with ones obtained before.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgment

The authors wish to deliver their sincere gratitude to the referee for constructive suggestions and technical comments on the paper.

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